LA-UR-15-21869
Approved for public release; distribution is unlimited.

Title: **MCNP Progress & Performance Improvements**

Author(s): Brown, Forrest B.
Bull, Jeffrey S.
Rising, Michael

Intended for: DOE NCSP Technical Program Review

Issued: 2015-03-14

DOE Nuclear Criticality Safety Program
Technical Program Review
18-19 March 2015

LA-UR-15-21869

# MCNP Progress
# &
# Performance Improvements

**Forrest B. Brown, Jeffrey S. Bull, Michael E. Rising**
**Monte Carlo Codes, XCP-3**
**Los Alamos National Laboratory**

Los Alamos NATIONAL LABORATORY EST.1943

Nuclear Criticality Safety Program

## US DOE/NNSA Nuclear Criticality Safety Program –

### What have we done for you lately (FY 2014, FY 2015) ?

- MCNP6.1.1 Release, with ENDF/B-VII.1
- Verification / Validation
- User Support & Training
- Performance Improvements
- Work in Progress

# MCNP6

# MCNP6 Status (1)

Monte Carlo Codes
XCP-3, LANL

- **MCNP6 releases by RSICC**

**MCNP6.1 – 2013, production version**
**MCNP6.1.1 – 2014, same criticality, faster, beta features for DHS**

**Nuclear Data – ENDF/B-VII.1 data, updates, & older data**
**Reference Collection – 700+ technical reports**
**V&V Test Collection – 1434 test problems**

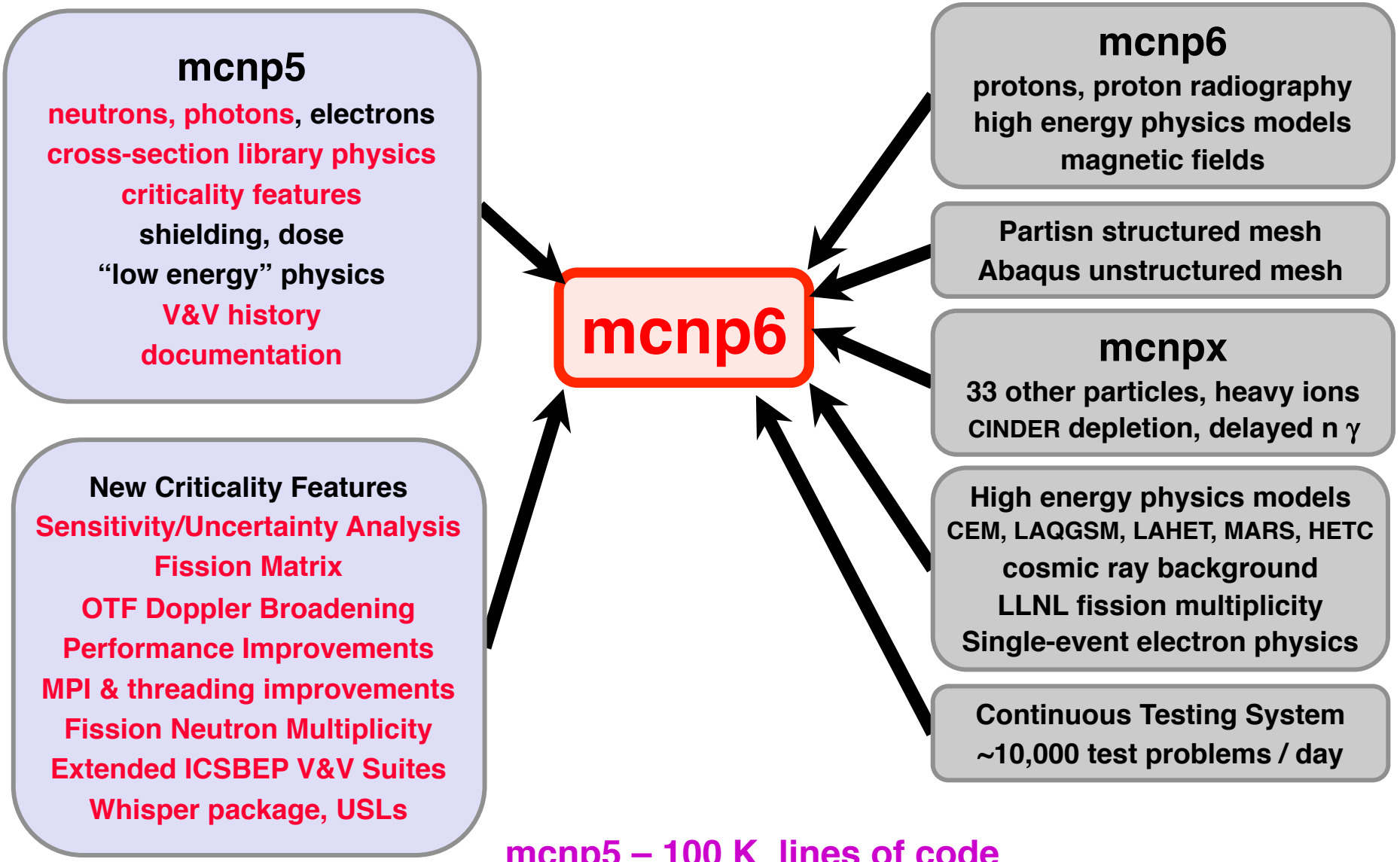
**12,000+ copies of MCNP5 distributed by RSICC**
**7,819+ copies of MCNP6 distributed by RSICC**

- **MCNP5 is frozen & unsupported. Last version 2010.**
- **Criticality safety community needs to transition to MCNP6**

Support from DOE-NNSA-NCSP, DOE-NNSA-ASC, DOE, DOD, DTRA, DHS/DNDO, NASA, & others

# MCNP6 Status (2)

Monte Carlo Codes
XCP-3, LANL




mcnp5 – 100 K lines of code

mcnp6 – 500 K lines of code

# Verification
# &
# Validation

# Verification & Validation (1)



## We do a lot of verification/validation work - all the time:

## MCNP Verification-Validation, 100+ reports on MCNP Website

**MCNP6 Optimization & Testing for Criticality Safety Calculations, LA-UR-15-20422 (2015).**

**Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems, LA-UR-14-23352 (2014).**

**Verification of MCNP6.1 & MCNP6.1.1 for Criticality Safety Applications, LA-UR-14-22480 (2014).**

**Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications**, LA-UR-13-22196 (**2013**).

**Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications**, LA-UR-12-210 (**2012**).

**MCNP5-1.60 Release & Verification**, Trans Am Nuc Soc 104, June 2011, LA-UR-11-00230 (**2011**).

**ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks & Reactor Experiments**, Nuclear Data Sheets, Vol 112, No. 12, 2997-3036 [LA-UR-11-11271] (**2011**).

**An Expanded Criticality Validation Suite for MCNP**, ICNC-2011, LA-UR-11-04170 (**2011**).

**Verification of MCNP5-1.60**, LA-UR-10-05611 (**2010**).

## Nuclear Data

**Listing of Available ACE Data Tables, LA-UR-13-21822, rev 4 (2014)**

**Continuous Energy Neutron Cross Section Data ...ENDF/B-VII.1**, LA-UR-13-20137 (**2013**).

**LANL Data Testing Support for ENDF/B-VII.**1, LA-UR-12-20002 (**2012**).

**ENDF/B-VII.1 Nuclear Data.....**, Nuclear Data Sheets, Vol 112, No. 12, 2887-2996 (**2011**).

**ENDF/B-VII.0: ... Nuclear Data** ..., Nuclear Data Sheets, Vol. 107, Number 12 (**2006**)

**New ACE-Formatted Neutron and Proton Libraries Based on ENDF/B-VII.0**, LA-UR-08-1999 (**2008**).

**Release of New MCNP S(α,β) Library ... ENDF/B-VII.0**, LA-UR-08-3628 (**2008**).

# Verification & Validation (2)

Monte Carlo Codes
XCP-3, LANL

Table 1. MCNP6.1 and MCNP6.1.1-Beta Results for Analytic Keff Benchmarks

| Case | Name | Analytic keff | MCNP_Results keff | std |
|---|---|---|---|---|
| prob11 | Ua-1-0-IN | 2.25000 | 2.25000 | 0.00000 |
| prob14 | Ua-1-0-SP | 1.00000 | 1.00006 | 0.00010 |
| prob18 | Uc-H2O(2)-1-0-SP | 1.00000 | 1.00005 | 0.00011 |
| prob23 | UD2O-1-0-CY | 1.00000 | 1.00000 | 0.00006 |
| prob32 | PUa-1-1-SL | 1.00000 | 0.99995 | 0.00011 |
| prob41 | UD2Ob-1-1-SP | 1.00000 | 1.00003 | 0.00007 |
| prob44 | PU-2-0-IN | 2.68377 | 2.68377 | 0.00003 |
| prob54 | URRa-2-0-SL | 1.00000 | 1.00007 | 0.00013 |
| prob63 | URRd-H2Ob(1)-2-0-ISLC | 1.00000 | 0.99993 | 0.00006 |
| prob75 | URR-6-0-IN | 1.60000 | 1.59999 | 0.00001 |

Results are identical for MCNP6.1 and MCNP6.1.1-Beta.

Wall-clock time, using 8 threads on Mac Pro:

MCNP6.1 151 min

MCNP6.1.1-beta 87 min

From LA-UR-14-22480

# Verification & Validation (3)



**From LA-UR-14-22480 (2014), using Intel-12 compiler for all codes:**

**VERIFICATION_KEFF Suite** – analytic problems with exact $K_{eff}$ results

- **MCNP6.1 & MCNP6.1.1:** **All results match**

**VALIDATION_CRITICALITY Suite** – 31 ICSBEP Cases, ENDF/B-VII.0

- **MCNP5, MCNP6.1, MCNP6.1.1:** **All results match**

**VALIDATION_CRIT_EXPANDED Suite** – 119 ICSBEP Cases, ENDF/B-VII.0

**Shortened Problems**

- **MCNP5, MCNP6.1, MCNP6.1.1:** **All results match**

**Standard Problems**

- **MCNP5, MCNP6.1, MCNP6.1.1:** **4 diffs, within statistics**

**VALIDATION_CRIT_WHISPER Suite** – **1086** ICSBEP Cases, ENDF/B-VII.1

- **Used for LANL NCS validation of MCNP6.1 & ENDF/B-VII.1, and determining baseline USLs for Pu-metal, -solution, & -oxide systems**
- **Includes sensitivity profiles for all reactions/isotopes/problems**
- **Will be added to standard MCNP Criticality V&V suites in 2015**

# Verification & Validation (4)



- **Very thorough testing of MCNP6.1 & MCNP6.1.1 on many computer platforms:**
  - **Brown, "MCNP6 Optimization & Testing for Criticality Safety Calculations", LA-UR-15-20422 (2015).**
  - **Brown, Kiedrowski, Bull, "Verification of MCNP6.1 & MCNP6.1.1 for Criticality Safety Applications", LA-UR-14-22480 (2014).**
  - **Brown, Kiedrowski, Bull, "Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications", LA-UR-13-22196 (2013).**

**Conclusion:** **MCNP6.1 & MCNP6.1.1 are solid & reliable for criticality safety calculations**

- **MCNP6.1 is 20-30% slower than MCNP5,**
  **MCNP6.1.1 is 10% faster than MCNP5**

# User Support
# &
# Training

# User Support & Training (1)

Monte Carlo Codes
XCP-3, LANL

- **User support**
  - **MCNP Forum - User-group, beginners & experts, >1000 members**
  - **MCNP Website, MCNP Reference Collection**
  - **Summer students**
  - **Direct hands-on support for LANL NCS Division**
  - **Email consulting to many crit-safety analysts**
- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP**
    - FY13: 3 classes (including special class for LANL NCS group certification)
    - FY14: 2 classes (with some LANL NCS staff)
    - FY15: 2 classes (with some LANL NCS & DOE/NNSA staff), possibly other sites
- **Conferences & Journals**
  - **M&C 2015, ICNC 2015, SNA+MC 2013**
  - **ANS Washington, Reno, Anaheim, San Antonio**
  - **OECD/NEA/WPNCS Expert Groups**
    - Advanced Monte Carlo Techniques, Sensitivity/Uncertainty

# Performance Improvements

# MCNP 2020 (1)



- **MCNP6.1**
  - Last few years – other developers focused on features, merger, testing, release
  - Slower, by 30-500 %
- **Path forward – MCNP 2020**
  - Concerted effort to modernize the codebase, upgrade foundations
  - Goals: faster, sustainable, flexible
  - Necessary for MCNP to survive into the 2020's & new computers
  - Proposed joint support by DOE-ASC & DOE-NCSP
    - Experienced Lead (Brown)
    - 2-3 core developers

## MCNP 2020

- **Improve performance**
  - Goal: 2X speedup within 2 years
- **Upgrade core MCNP6 software**
  - Restructure, clean up coding, Fortran 2003 & C/C++ standards
  - Reorganize data structures
  - Evolution, not revolution
  - Reduce future costs for new development & maintenance
  - Goal: sustainable code
- **Prepare for future**
  - New computers – massive parallel, but less memory per core
  - Improve MPI & thread parallelism
  - Goal: flexible, adaptable code

# MCNP 2020 - Performance Improvements (2)

Monte Carlo Codes XCP-3, LANL

- **Initial 3-month effort, focus on speedup & optimization**
  - Focus on neutron criticality problems common to ASC & NCSP applications
  - Speedup factors from recent performance improvements, mcnp6.1.1:

**Performance Test Set**

| Criticality | | Other | |
|---|---|---|---|
| ks1 | 1.76 | void1 | 3.03 |
| ks2 | 2.13 | void2 | 4.11 |
| ks3 | 1.35 | void2 | 4.11 |
| ks4 | 1.36 | void3 | 2.72 |
| baw1 | 2.19 | det1 | 1.67 |
| baw2 | 1.59 | med1 | 1.15 |
| fvf | 2.04 | pht1 | 1.22 |
| g1 | 1.14 | | |
| g2 | 2.20 | | |
| pin | 1.73 | | |

**VALIDATION_CRITICALITY Suite**

Measured wall-clock times, including data I/O:

| | | |
|---|---|---|
| mcnp5 | release | 34.7 min |
| mcnp6.1 | release | 43.9 min |
| mcnp6.1.1 | NEW | 27.9 min |

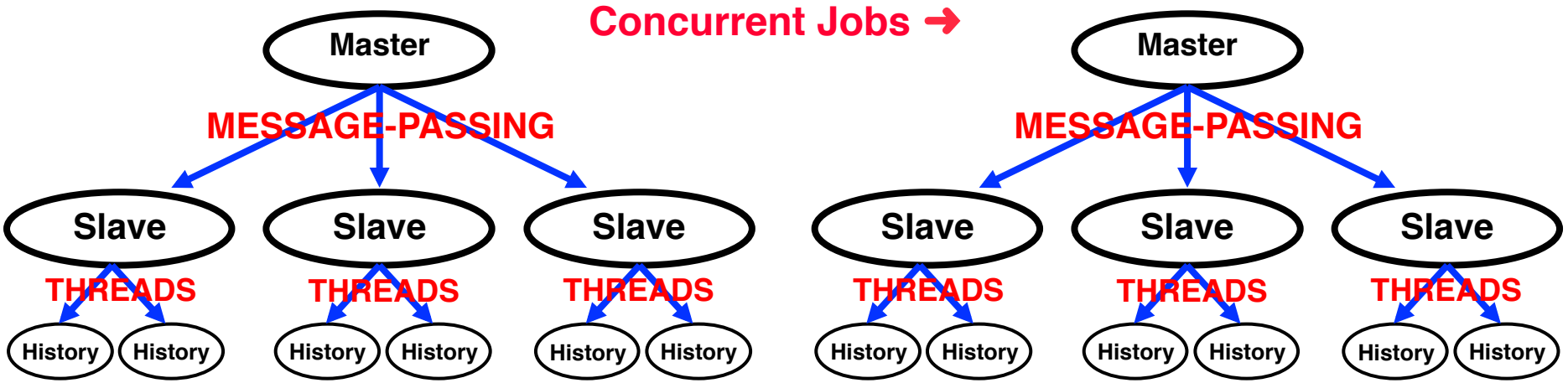
➜ 1.57 X speedup over mcnp6.1
➜ 1.24 X speedup over mcnp5

**Performance Benchmark Suite**

Speedups vs MCNP6.1 Release

| Neutron Problems | Speedup |
|---|---|
| BAWXI2 | 4.37 |
| GODIVA | 1.05 |
| Mode n in air w 750,000 tally bins | 1.18 |
| Well log problem | 1.91 |
| 100M lattice cells in void | 5.17 |
| **Other** | |
| mode p e in air | 1.01 |
| mode n p e in air | 1.05 |
| mode p in air | 1.20 |
| Pulse height tally | 1.20 |
| Radiography | 1.07 |

## MCNP – Hierarchical Parallelism – Since 2000




## Parallel Processes

- **Total processes = (# jobs) x (# MPI processes) x (# threads)**
- **Tradeoffs:**
  - **More MPI processes - lots more memory & messages**
  - **More threads - contention from lock/unlock shared memory**
  - **More jobs - system complexity, combining results**

# MCNP 2020 - Performance Improvements (4)

Monte Carlo Codes XCP-3, LANL

## Run Times for VALIDATION_CRITICALITY Suite on Various Computers

| Computer | CPU Speed (GHz) | Mem. Speed (GHz) | Processors, Cores | MCNP Threads used | MCNP Version | Total Time (minutes) |
|---|---|---|---|---|---|---|
| MacBook 2010 | 2.7 | 1.1 | 1 - i7, 2 x 2 HT | 4 | mcnp6.1.1 | 88 |
| MacBook 2013 | 3.0 | 1.6 | 1 - i7, 2 x 2 HT | 4 | mcnp5-1.60 | 40 |
| | | | | 4 | mcnp6.1 | 62 |
| | | | | 4 | mcnp6.1.1 | 42 |
| Mac Pro 2010 | 3.0 | 0.67 | 2 - Xeon, 4 | 8 | mcnp5-1.60 | 30 |
| | | | | 8 | mcnp6.1 | 44 |
| | | | | 8 | mcnp6.1.1 | 28 |
| Windows 2012 | 2.7 | 1.3 | 2 - Xeon, 6 | 10 | mcnp6.1.1 | 19 |
| Mac Pro 2012 | 2.4 | 1.07 | 2 - Xeon, 4 x 2 HT | 16 | mcnp5-1.60 | 25 |
| | | | | 16 | mcnp6.1 | 32 |
| | | | | 16 | mcnp6.1.1 | 22 |
| Mac Pro 2014 | 2.7 | 1.6 | 1 - Xeon, 12 x 2 HT | 12 | mcnp5-1.60 | 14 |
| | | | | 12 | mcnp6.1 | 20 |
| | | | | 12 | mcnp6.1.1 | 14 |
| | | | | 14 | mcnp6.1.1 | 12 |

# Work in Progress

**Sensitivity/Uncertainty Methods**

**Whisper – Validation & USLs**

**MCNP 2020 – Near-Term Targets**

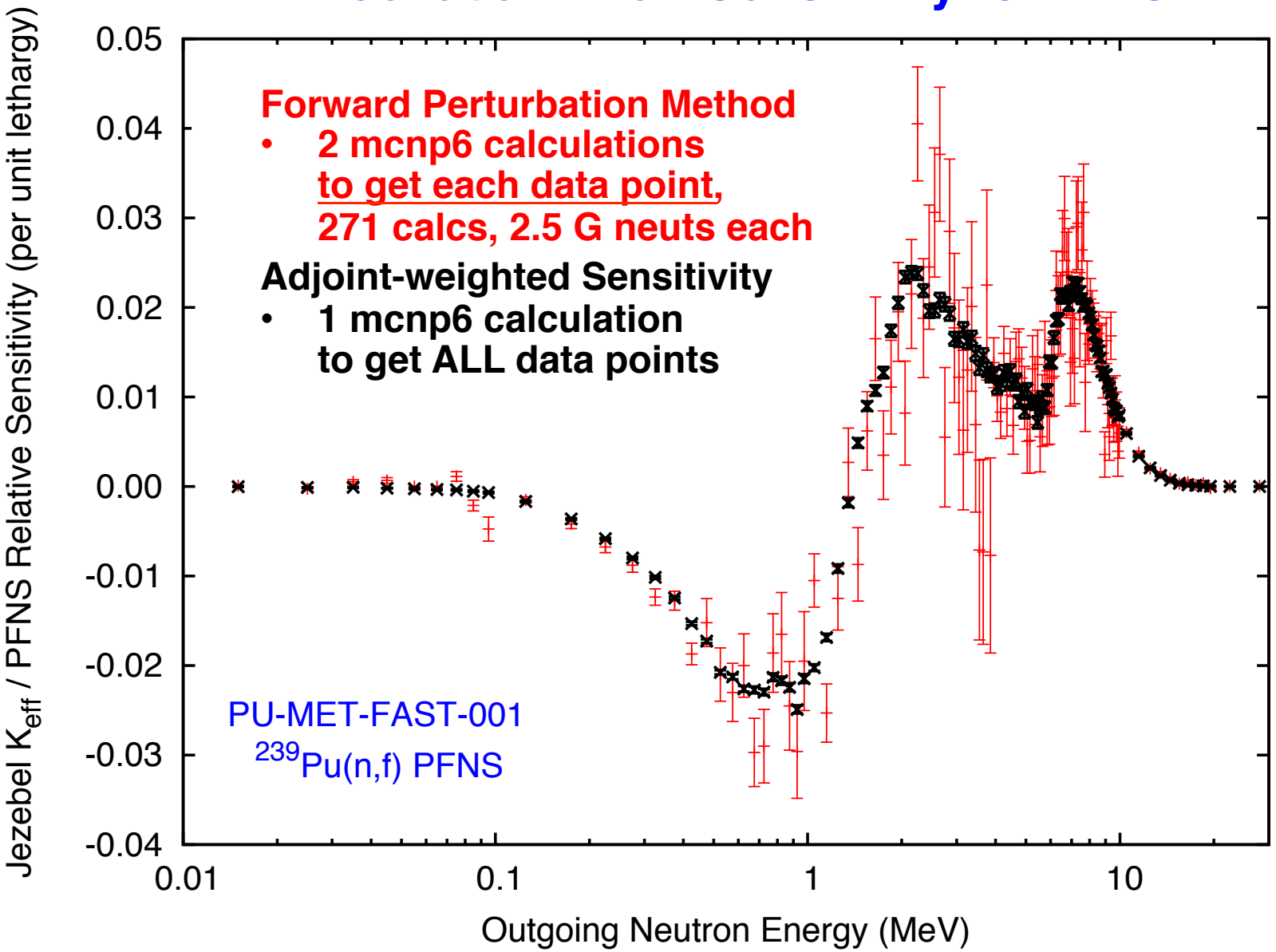
**Other R&D Work, with Universities**

# MCNP6 Sensitivity/Uncertainty (1)

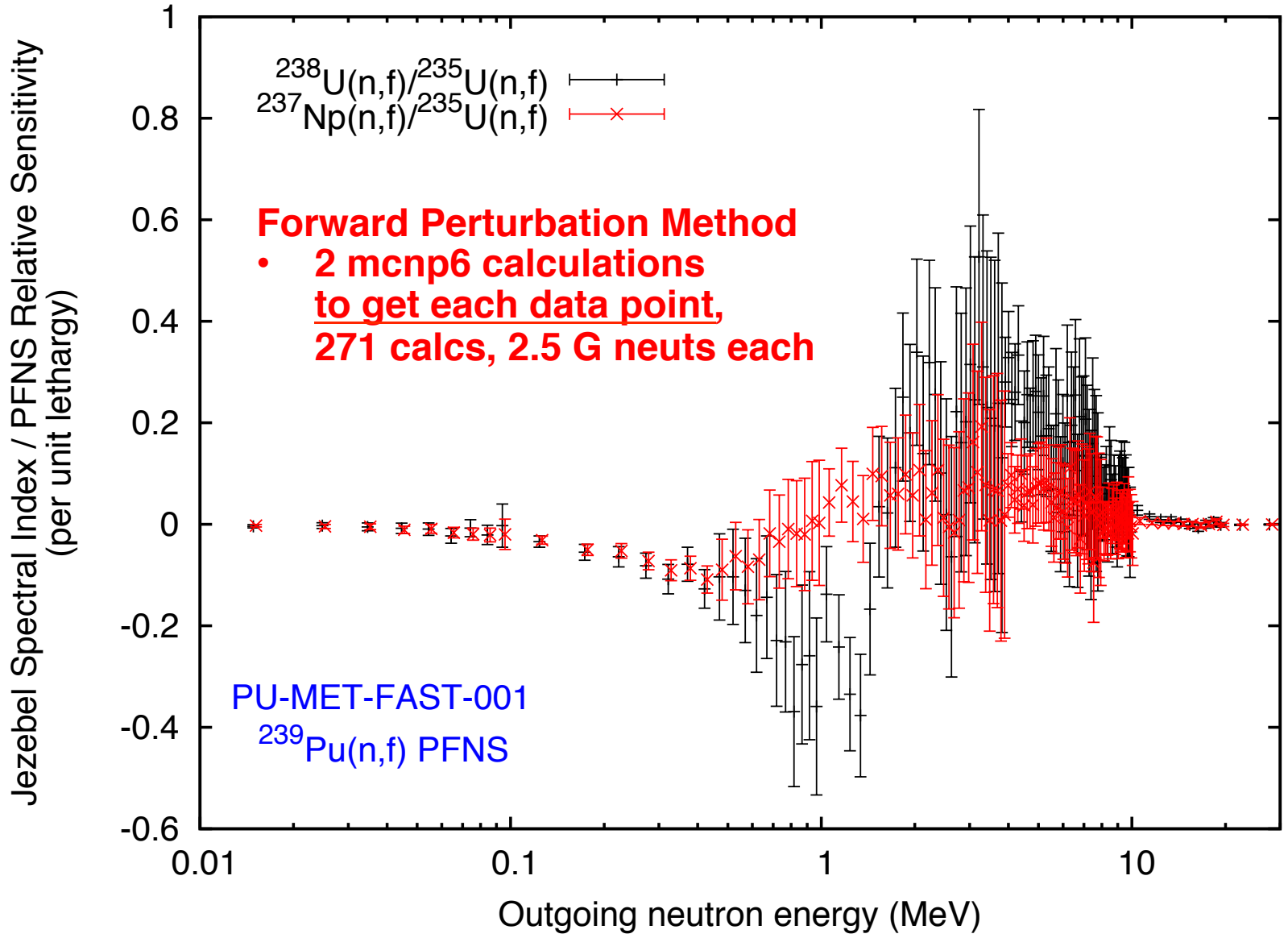


- **Adjoint-weighted sensitivity coefficient tallies can be used to predict the impact on Keff due to newly evaluated nuclear data**
- **With a recent evaluation of the $^{239}$Pu(n,f) prompt fission neutron spectrum (PFNS), we can quickly validate this new data against criticality safety benchmark simulations**
  - **Adjoint-weighted sensitivity calculation**
    - 1 MCNP6 calculation for adjoint-weighted results at all energy points in the sensitivity energy range
- **Some alternative approaches give poor results with more computational cost**
  - **Forward perturbation method**
    - Direct, simple, brute force – subtract base case & perturbed case for each energy point in the sensitivity energy range
    - Requires 100s or 1000s of separate MCNP calculations, with small statistics
    - Examples on next slides required 2 mcnp6 calculation for each data point, 271 calculations with 2.5 G neutrons each

# Jezebel – Keff Sensitivity to PFNS



# Jezebel – Spectral Indices Sensitivity to PFNS



# MCNP6 Sensitivity/Uncertainty (4)



- Other integral & semi-integral data have been measured on critical experiments such as,
  - A variety of spectral indices (ratios of reaction rates)
  - Overall and energy-dependent leakage

- When new nuclear data libraries are released (along with covariances), we should always
  - compare the calculated Keff to experiment
  - compare the calculated spectral indices, leakages, etc., against experiment to provide feedback to the nuclear data community

- MCNP6 needs to be able to compute adjoint-weighted sensitivity tallies for quantities other than keff, such as spectral indices, to compare against this other experimentally measured criticality experiment data because the alternative approaches perform very poorly in comparison

- This capability is under development. May be especially important for supporting the CIELO nuclear data evaluations.

# Whisper Methodology for Validation & USLs (1)

Monte Carlo Codes XCP-3, LANL

- **In early 2014, the XCP-3 & NCS groups at LANL undertook a major upgrade to the criticality safety computational capabilities**
  - **Previous: mcnp5-1.25, endf 4, 5, 6 (very old & unsupported)**
  - **Upgrade: mcnp6.1 + endf/b-vii.1, HPC cluster**
  - **Participants:**
    - Kiedrowski, Conlin, Favorite, Kahler, Kersting, Parsons, Walker, Brown, etc.
  - **References**
    - LA-UR-14-26558, *Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits*
    - LA-UR-14-26436, *User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation*
    - LA-UR-14-23202, *Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation*
    - LA-UR-14-23352, *Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems*

# Whisper Methodology for Validation & USLs (2)

Monte Carlo Codes XCP-3, LANL

- **Whisper ICSBEP Benchmark Suite**
  - **1086 ICSBEP benchmark problems from Mosteller, Kahler, others**
  - **Sensitivity profiles from adjoint-weighting for all isotopes/reactions/benchmarks**
- **Whisper methodology –** LA-UR-14-26558, LA-UR-14-26436, LA-UR-14-23352
  - **Verification of computer code system**
    - Installation tests, VERIFICATION_KEFF tests, config control, static linked, etc.
  - **Validation benchmarks**
    - Estimate missing uncertainties
    - Reject inconsistent benchmarks via iterated diagonal chi-squared method (~12%)
    - Correlation data from DICE; covariance data from ORNL (10% diag for missing)
    - Automated benchmark selection for AOA problem using sensitivity data to determine $C_k$ values; $C_k$ values used for weighting
  - **Calculational Margin**
    - Determine bias from non-parametric method based on Extreme Value Theory, using weighting determined from $C_k$ values
    - Determine bias uncertainty numerically from distribution of worst-case $k_{eff}$ bias
  - **Margin of Subcriticality**
    - Margin of 0.0050 for unknown code errors (expert judgment)
    - Margin for nuclear data uncertainty from GLLS method
    - Additional margin – analyst judgment for AOA & problem, conservatism, etc.
  - **USL = 1.0 – Calculational Margin – Margin of Subcriticality**

# Whisper Methodology for Validation & USLs (3)



- **Current activities**
  - **NCS Division SQM for Whisper (XCP-3 assisting in review)**
    - *NCS-SQM Whisper Code Inspection (Sartor, in preparation)*
    - *NCS-SQM Whisper Verification & Validation (Sartor, in preparation)*
    - *NCS-SQM MCNP6 KCODE Verification & Validation (Sartor, in preparation)*
  - **Whisper software**
    - Potential use at other DOE sites
    - Well-documented and tested alternative to tsunami/tsurfer/etc
    - **To be included with standard MCNP6 distribution through RSICC**
  - **Whisper benchmark suite**
    - MCNP input for 1086 ICSBEP benchmarks
    - Valuable resource for all MCNP criticality-safety users & sites
    - **To be included with standard MCNP6 distribution through RSICC**
  - **Improved covariance data – produce with NJOY & new ACE formats**
    - **Minor mods to Whisper, when Nuclear Data Team produces improved data**
  - **Whisper training**
    - **Proposed to DOE-NCSP for LANL & other DOE crit-safety groups**
    - Local training at LANL (not DOE-NCSP funded)

# MCNP 2020 – Near-Term Targets

Monte Carlo Codes
XCP-3, LANL

## NCSP-Related

- **Parallel threading** – measure 2015 performance of atomic-operations vs critical-sections
- **List tallies** – alternative tally scheme, to save memory & reduce lock/unlock overhead for threading
- **Light-weight cycle rendezvous for MPI calculations** – reduce unnecessary MPI messaging
- **Compliance with Fortran-2003 standard** – eliminate all coding using older or nonstandard features
- **Fission neutron multiplicity** – restructure & combine, ensure correct threading

## Depending on non-NCSP funding

- **MPI improvements** – nonblocking messages, asynchronous transfers, in-place transfers, improved interface using Fortran-2003 polymorphism
- **Examine memory allocation** – rearrange for better cache utilization
- **Tally servers** – remote node storage for tallies with very large memory requirements
- **New standardized dump file** – direct access, access by dataset name, etc.
- **Upgrade for PTRAC & SSR** – permit use in parallel calculations, not just serial
- **HDF5 &/or MPI-IO** – improve read/write speed & portability of file output

# Other R&D work, with Universities

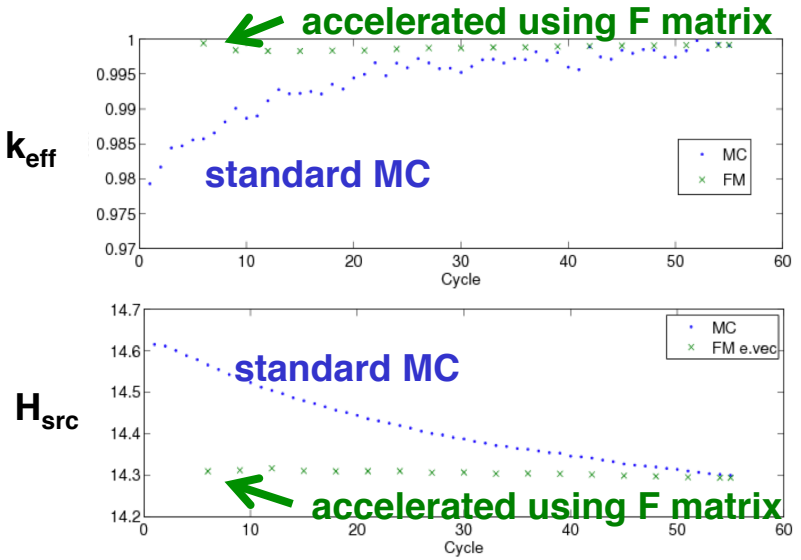
Monte Carlo Codes
XCP-3, LANL

## Physics & Temperature Dependence

- Full temperature dependence of S(a,b) thermal scattering (RPI)
- Unresolved resonances (MIT)
- Implement modified free-gas scatter, to model resonance upscattering for epithermal neutrons (Michigan)
- Investigate coupling MCNP into multiphysics calculations (Michigan)
- V&V for using explicit fission neutron multiplicity distributions in criticality calculations (New Mexico)
- Doppler coefficients (New Mexico)

## Fission Matrix

- Forward & adjoint methods, sparse matrix schemes (Michigan)
- Automatically determine source convergence, without user input
- Apply to subcritical multiplication problems
- Accelerate source convergence



# Summary



- MCNP6.1, MCNP6.1.1, & ENDF/B-VII.1 released
- Next release – TBD, probably FY 2016

- Impact on Criticality Calculations ➜ none
  - All basic KCODE criticality features same as for MCNP5
  - Matches results with MCNP5 for criticality suites

- MCNP6 speed improved by 1.2 – 4 X for crit-safety.
- More MCNP 2020 improvements in progress

- Sensitivity/uncertainty methods based on adjoint-weighted tallies are being used routinely in many areas
  - Outstanding success due to long-range vision & support from NCSP

- Whisper methodology for validation & USLs is important to LANL NCS, and to other DOE sites

- Criticality-safety community needs to transition to MCNP6 over the next few years

# Questions ?